# Interference effects in interacting quantum dots

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In this paper we study the interplay between interference effects in quantum dots (manifested through the appearance of Fano resonances in the conductance), and interactions taken into account in the self-consistent Hartree-Fock approximation. In the non-interacting case we find that interference may lead to the observation of more than one conductance peak per dot level as a function of an applied gate voltage. This may explain recent experimental findings, which were thought to be caused by interaction effects. For the interacting case we find a wide variety of different interesting phenomena. These include both monotonous and non-monotonous filling of the dot levels as a function of an applied gate voltage, which may occur continuously or even discontinuously. In many cases a combination of the different effects can occur in the same sample. The behavior of the population influences, in turn, the conductance lineshape, causing broadening and asymmetry of narrow peaks, and determining whether there will be a zero transmission point. We elucidate the essential role of the interference between the dot levels in determining these outcomes. The effects of finite temperatures on the results are also examined.

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## I. INTRODUCTION

Transport in quantum dots has been the topic of an intense scrutiny for more than twenty years (for a review, see, e.g., Ref. 1). However, most of both experimental and theoretical studies were concentrated on either of the two limits: (a) the limit of strong dot-lead coupling ("open dots"), in which the discreteness of the dot's energy spectrum is completely lost; (b) the limit of weak dot-lead coupling ("closed dots"), in which, due to the Coulomb Blockade, each of the dot's levels creates a well defined peak in the dependence of the dot's conductance on an applied gate voltage.

In recent years, focus has shifted to the intermediate coupling case. In this case, dot-lead coupling is weak enough so that the dot's energy spectrum cannot be considered as a continuum, but there are interference effects between different dot levels, manifested through the appearance of Fano resonances in the dot's conductance[2,3].

Most the theoretical studies have so far concentrated on interference effects in non-interacting dots[4,5,6]. However, recent experimental findings[7] indicate that interplay between Fano resonances and electron-electron interactions may lead to interesting new effects.

Recently, there have been some attempts to understand the intermediate coupling regime. Some of these efforts[8,9] were confined to the case were only one dot level is coupled to the leads, so that no interference can occur; while others[10,11,12,13,14,15] discussed only a limited range of the parameter space, (and thus did not mention, e.g., the possibility of discontinuities for finite width levels), or considered solely the question of the transmission phase[16], not emphasizing the behavior of the dot's population and its conductance. In this paper we try to address those unexplored questions.

We discuss both the linear electric conductance, which is the most easily accessible quantity experimentally, and the occupation of the dot, which can be probed by, e.g., coupling it electrostatically to a quantum point-contact. In fact, our model of a dot with several levels can also describe a system of single level dots connected in parallel, so that the occupation of each level can be measured separately.

After introducing out model and calculation methods in Sec. II, we briefly examine the non-interacting Fano resonance in Sec. III, and show that the observations by Johnson *et al.*[7], interpreted by them as interacting Fano resonances, can be explained as the result of interference between one wide level and many narrow levels in a non-interacting system.

In Sec. IV we move to include interactions, which are treated in a Hartree-Fock approximation. We show that many new effects occur. The interactions may lead to a non-monotonous filling of each level as a function of an applied gate voltage. The dependence on the gate voltage may be discontinuous, even when *all* the dot's levels have finite widths. In many cases both continuous and discontinuous non-monotonicity can occur in the same case. We find how the behavior of the population affects the conductance. Interference effects between the dot levels play a very important role in determining which type of behavior will occur in a given sample. We also discuss the effects of finite temperatures on the results, which is essential for analyzing experimental data.

We conclude by reviewing our main findings in Sec. V.

## II. MODEL AND METHODS OF CALCULATION

We consider the following model Hamiltonian, describing spinless electrons (experimentally realizable by applying a strong in-plane magnetic field) moving in a system composed of a (possibly interacting) dot and non-interacting leads:

$$\hat{H} = \hat{H}_D + \hat{H}_L + \hat{H}_R + \hat{H}_T. \tag{1}$$

This Hamiltonian is composed of three parts:

I. The quantum-dot Hamiltonian:

$$\hat{H}_D = \sum_i \epsilon_{i,v} \hat{a}_i^\dagger \hat{a}_i + \frac{U}{2} \sum_{i \neq j} \hat{a}_i^\dagger \hat{a}_i \hat{a}_j^\dagger \hat{a}_j. \tag{2}$$

Here $\hat{a}_i$ and $\hat{a}_i^\dagger$ are creation and annihilation operators, respectively, of an electron in the dot's $i$'th level; $\epsilon_{i,v} = \epsilon_i - eV_g$ is the corresponding single-particle energy, modified by an applied gate voltage $V_g$ ($e$ is the absolute value of the electronic charge); and $U = e^2/C$ is the strength of interaction between electrons in the dot, assumed to consist simply of a charging energy.

II. The Hamiltonian of lead $\ell$ ( $= L$ or $R$ for the left or right lead, respectively):

$$\hat{H}_\ell = \sum_k \epsilon_{k,\ell} \hat{c}_{k,\ell}^\dagger \hat{c}_{k,\ell}, \tag{3}$$

where $\hat{c}_{k,\ell}^\dagger, \hat{c}_{k,\ell}$ are creation and annihilation operators of an electron in the $\ell$'th leads $k$'th mode, $\epsilon_{k,\ell}$ the corresponding single-particle energy. In the following we assume that each lead is a band of width $2D$, (much larger than any other energy scale in the system), and constant density of states.

III. The tunneling Hamiltonian:

$$\hat{H}_T = \sum_{i,k,\ell} \left( t_{k,\ell}^i \hat{a}_i^\dagger \hat{c}_{k,\ell} + H.C. \right), \tag{4}$$

where the tunneling matrix elements $t_{k,\ell}^i$ are assumed real (i.e., there is no applied out-of-plane magnetic field), and independent of $k$. It is also assumed that $\left|t_L^i\right| = \left|t_R^i\right|$.

For $U = 0$ (the non-interacting case), the Hamiltonian can be exactly solved. The matrix elements (in the dot states space) of the inverse retarded (advanced) Green function for the dot states is given by:

$$\left(G(\epsilon)^{r,a}\right)_{i,j}^{-1} = \epsilon - \epsilon_{i,v}\delta_{i,j} \pm \frac{i}{2} \sum_{\ell=R,L} \Gamma_{i,j}^\ell, \tag{5}$$

where $\Gamma_{i,j}^\ell$, the matrix elements of the width of the dot's levels due to their coupling with lead $\ell$, are given by:

$$\Gamma_{i,j}^\ell = 2\pi \left(t_\ell^i\right)^* t_\ell^j \rho_\ell, \tag{6}$$

$\rho_\ell$ being the density of states in the $\ell$'th lead. Thus, $\left(\Gamma_{i,j}^\ell\right)^2 = \Gamma_{i,i}^\ell \Gamma_{j,j}^\ell$. In addition, by the above assumptions on the tunneling matrix elements, $\left|\Gamma_{i,j}^L\right| = \left|\Gamma_{i,j}^R\right|$. Thus, one is free to choose the diagonal matrix elements of $\Gamma^L$, and the *signs* of the off-diagonal elements of both $\Gamma^L$ and $\Gamma^R$. In the following we will denote the total width, $\Gamma_L + \Gamma_R$ by $\Gamma$, and its $i$'th diagonal matrix elements by $\Gamma_i$.

Using the dot's Green functions, one can find the following averages, related to the average occupation of the dot's states at temperature $T$:

$$\langle \hat{a}_i^\dagger \hat{a}_j \rangle = -\frac{1}{\pi} \int_{-D}^{D} f(\epsilon) \Im\{G_{i,j}^r(\epsilon)\} d\epsilon, \tag{7}$$

$f(\epsilon) = 1/(\exp[(\epsilon - \mu)/T] + 1)$ being the Fermi-Dirac distribution function with chemical potential $\mu$ and temperature $T$, using units where Boltzmann's constant equals unity. In particular, the average occupation of the dot's $i$'th level is $n_i = \langle \hat{a}_i^\dagger \hat{a}_i \rangle$.

We can also find the linear conductance, following Meir and Wingreen[17]:

$$g = \frac{e^2}{h} \int_{-D}^{D} [-f'(\epsilon)] \mathrm{Tr}\left[G^r(\epsilon)\Gamma_L G^a(\epsilon)\Gamma_R\right] d\epsilon. \tag{8}$$

The interacting case ($U \neq 0$) is treated using the self-consistent Hartree-Fock approximation. This amounts to replacing the dot Hamiltonian (2) by an effective single-particle Hamiltonian, given by:

$$\begin{aligned} \hat{H}_D^{eff} &= \sum_i \left( \epsilon_{i,v} + U \sum_i n_i \right) \hat{a}_i^\dagger \hat{a}_i - U \sum_{i,j} \langle \hat{a}_i^\dagger \hat{a}_j \rangle \hat{a}_j^\dagger \hat{a}_i \\ &\quad - \frac{U}{2} \left( \sum_i n_i \right)^2 + \frac{U}{2} \sum_{i,j} \langle \hat{a}_i^\dagger \hat{a}_j \rangle^2. \end{aligned} \tag{9}$$

The diagonal terms in this expression are the Hartree contribution, while Fock correction leads to the off-diagonal terms. Using Eqs. (5) and (7), the problem is reduced to solving a set of self-consistent equations for the averages $\langle \hat{a}_i^\dagger \hat{a}_j \rangle$. One can show that the Fock terms vanish for any pair of levels $i, j$ for which $\Gamma_{i,j}^L = -\Gamma_{i,j}^R$.

In many cases there are several solutions to the Hartree-Fock equations, corresponding to different dot states being almost full or almost empty. In those cases one should average over the solutions, giving each a probability factor proportional to $\exp(-\Omega/T)$, where $\Omega$ is the grand canonical free energy:

$$\Omega = \frac{T}{\pi} \int_{-D}^{D} \ln\left[1 + e^{\frac{\mu - \epsilon}{T}}\right] \Im\{\mathrm{Tr}\left[G^r(\epsilon)\right]\} d\epsilon. \tag{10}$$

In particular, at zero temperature only the solution with the lowest chemical potential should be retained.

We mention in passing that the above integrals for the free energy, occupations and conductance can be expressed in terms of the logarithm of the gamma function of a complex argument and its first two derivatives (the digamma and trigamma functions)[18], respectively, to facilitate faster computation.

## III. INTERFERENCE EFFECTS IN NON-INTERACTING DOTS

We first consider the non-interacting case. Here, for a two-level dot, there are two possibilities, depending on

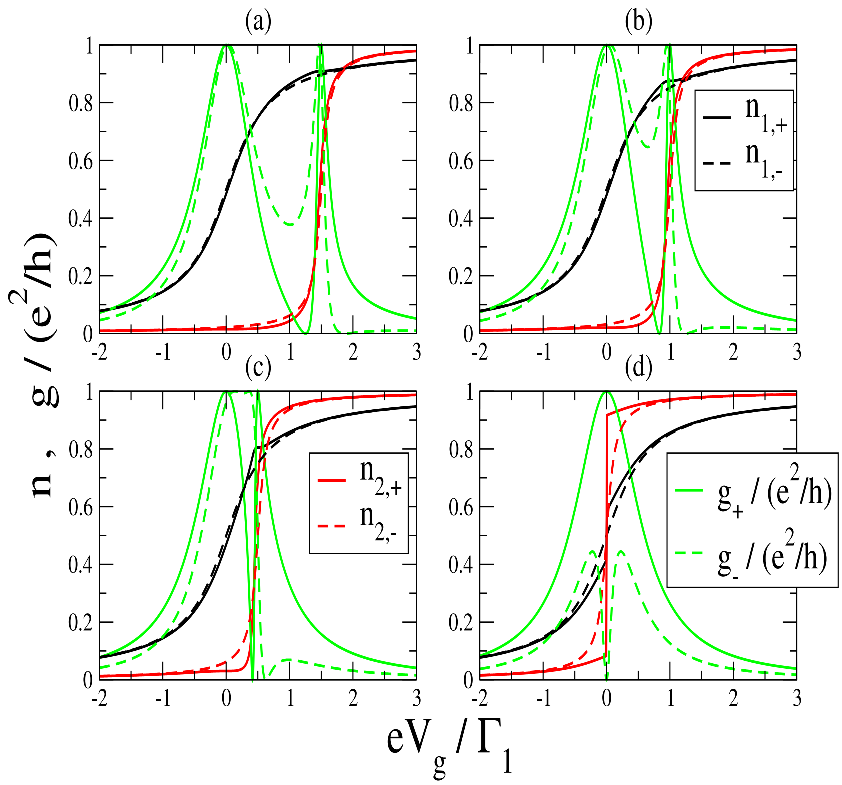


FIG. 1: Level occupations and conductance of a two-level non-interacting dot at zero temperature. In all the graphs, $\epsilon_1/\Gamma_1 = 0.0$, $\Gamma_2/\Gamma_1 = 0.2$, while $\epsilon_2$ varies: (a) $\epsilon_2/\Gamma_1 = 1.5$; (b) $\epsilon_2/\Gamma_1 = 1.0$; (c) $\epsilon_2/\Gamma_1 = 0.5$; (d) $\epsilon_2/\Gamma_1 = 0.0$.

the relative signs of the matrix elements of the widths $\Gamma_{R,L}$ between the two states. These will be termed the plus (minus) configuration for positive (negative) sign of $\Gamma^R_{1,2}/\Gamma^L_{1,2}$. If we make a transformation from the lead operators $\hat{c}_{k,R}, \hat{c}_{k,L}$ to the combinations $\hat{c}_{k,\pm} = (\hat{c}_{k,R} \pm \hat{c}_{k,R})/\sqrt{2}$, we find that in the plus case the two dot states are connected to the $\hat{c}_{k,+}$ states, whereas in the minus case one dot state is connected to the $\hat{c}_{k,+}$ states, while the other is connected with the $\hat{c}_{k,-}$ states. Thus, in the plus case the two dot states are effectively coupled to a single lead, while in the minus case each dot state is connected to a different effective lead[11].

The local density of states of each level, $\rho_i$, is given by ($i'$ is the index of the other level):

$$\rho_i^+(\epsilon) = \frac{1}{\pi}\frac{\frac{\Gamma_i}{2}(\epsilon-\epsilon_{i',v})^2}{(\epsilon-\epsilon_{i,v})^2(\epsilon-\epsilon_{i',v})^2+\left(\frac{\Gamma_i+\Gamma_{i'}}{2}\right)^2(\epsilon-\epsilon_{+,v})^2}, \tag{11a}$$

$$\rho_i^-(\epsilon) = \frac{1}{\pi}\frac{\frac{\Gamma_i}{2}}{(\epsilon-\epsilon_{i,v})^2+\left(\frac{\Gamma_i}{2}\right)^2}, \tag{11b}$$

where $\epsilon_{\pm,v} = (\Gamma_1\epsilon_{2,v} \pm \Gamma_2\epsilon_{1,v})/(\Gamma_1 \pm \Gamma_2)$. As one can see, in the minus case, the density of states of each of the dot's levels is unaffected by the other level, because they are effectively decoupled, as was explained above. Thus, their populations follow the usual $n_i = 1/2 + \tan^{-1}[(\mu-\epsilon_{i,v})/(\Gamma_i/2)]/\pi$ low. However, in the plus case, the levels interfere. As a result, the local density of states of each level goes to zero at the position of the other level. Thus, as the two levels approach each other, the density of states for both levels develops a sharp peak, going from zero to its maximum in a gate voltage distance which goes as $|\epsilon_1-\epsilon_2|$, instead of the widths $\Gamma_i$. This causes the populations $n_i$ to vary fast for $V_g$ between the two level energies. When the level energies exactly coincide, this sharp feature becomes a delta function peak in the density of states, or a discontinuous jump in the level population as a function of the gate voltage. Indeed, in this latter case, due to the degeneracy of the dot levels, one can transform to a basis of the states where one level is totally decoupled from the leads[4,10].

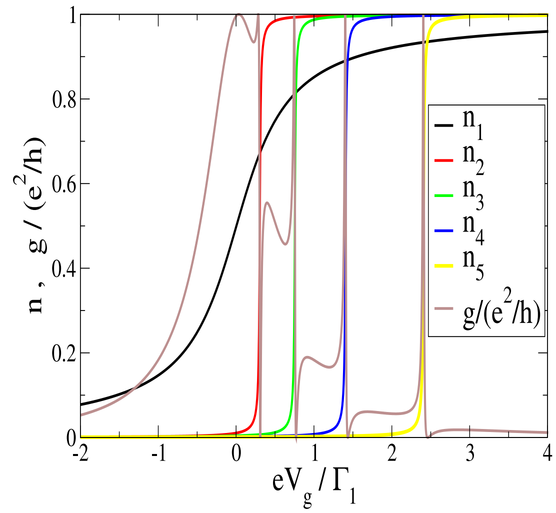


FIG. 2: Level occupations and conductance of a non-interacting dot with a single broad level and four narrow levels, at zero temperature. The wide level is coupled to one of the leads with a sign opposite to that of the narrow levels. The levels are at $\epsilon_i/\Gamma_1 = \{0.0, 0.3, 0.75, 1.4, 2.4\}$, with widths $\Gamma_i/\Gamma_1 = \{1.0, 0.02, 0.02, 0.02, 0.02\}$, for i=1...5. The general shape of the conductance function resembles Fig. 1 of Ref. 7.

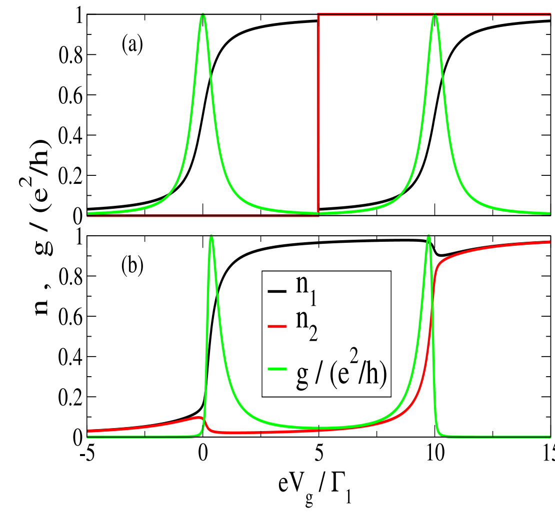


FIG. 3: The two basic phenomena of non-monotonic charging. The graph shows level occupations and conductance of a two-level interacting dot at zero temperature. The two levels are connected in the minus configuration. In both graphs, $\epsilon_1/\Gamma_1 = 0.0$, $U/\Gamma_1 = 10.0$. (a) effect I: $\epsilon_2/\Gamma_1 = 0.0$, $\Gamma_2/\Gamma_1 = 0.0$; (b) effect II: $\epsilon_2/\Gamma_1 = 0.1$, $\Gamma_2/\Gamma_1 = 1.0$. Consult the text for further explanation.

The conductance in each case is given by:

$$g^+ = \frac{e^2}{h}\frac{\left(\frac{\Gamma_1+\Gamma_2}{2}\right)^2(\mu-\epsilon_{+,v})^2}{(\mu-\epsilon_{1,v})^2(\mu-\epsilon_{2,v})^2+\left(\frac{\Gamma_1+\Gamma_2}{2}\right)^2(\mu-\epsilon_{+,v})^2}, \tag{12a}$$

$$g^- = \frac{e^2}{h}\frac{\left(\frac{\Gamma_1-\Gamma_2}{2}\right)^2(\mu-\epsilon_{-,v})^2}{\left[(\mu-\epsilon_{1,v})^2+\left(\frac{\Gamma_1}{2}\right)^2\right]\left[(\mu-\epsilon_{2,v})^2+\left(\frac{\Gamma_2}{2}\right)^2\right]}. \tag{12b}$$

Since conductance occurs by transmission of electrons between the left and right leads, and not between the $\hat{c}_{k,\pm}$ combinations, we find interference effects in the conductance in *both* cases. Thus, in the plus case, the conductance reaches its maximal possible value (of $e^2/h$) when the $\mu$ equals one of the dot's levels ($\epsilon_1$ or $\epsilon_2$), and goes to zero for $\mu = \epsilon_+$, i.e., between the conductance peeks. In the minus case, the conductance reaches its maximal value for $\mu$ in the vicinity of (but slightly different from) the dot's levels. It goes to zero at $\mu = \epsilon_-$, which lies outside the peaks. When $\epsilon_1$ and $\epsilon_2$ are sufficiently different, the conductance reaches its maximal possible value of $e^2/h$ at the peaks. When the dot's levels are too close the two peaks near the level energies become smaller, and eventually merge into a single peak. Finally, For $\epsilon_1 = \epsilon_2$ and $\Gamma_1 = \Gamma_2$, there is a complete destructive interference between the two levels, and $g = 0$ for all $\mu$ values.

All the above results are exemplified in Fig. 1. Here, and in the following, we set $\mu = 0$, and vary the gate voltage $V_g$. One can see that the interference effects result in an asymmetric shape of the conductance peaks, usually referred to as "Fano Resonances"[2,3,5,6,7].

We note that if the couplings to the left and right leads were different in magnitude, we would get the same qualitative picture, but the conductance would have reached values lower than $e^2/h$ even at the peaks in all cases.

One can show the above results for the conductance obey the the relation $g^\pm = e^2/h \times \sin^2[\pi(n_1 \pm n_2)]$ at zero temperature; this relation is also obeyed in the interacting case, in our Hartree-Fock approximation. The validity of this equation is, however, much wider, since it is required by the Friedel sum rule[19,20].

As one can see, in the minus case, we get three conductance peaks from only two dot levels. As we show in Fig. 2, this can be extended to the case of many narrow levels and a single wide level, where the latter's coupling to one of the the leads has an opposite sign (in the sense discussed above) to that of the narrow levels. In this way we get two peaks in the conductance for each narrow levels. The conductance curve is very similar to some of the experimental results of Johnson *et el.*[7]. This shows that interference effects alone can qualitatively explain the experiments, without the need to resort to interaction effects, as was done by the above mentioned authors.

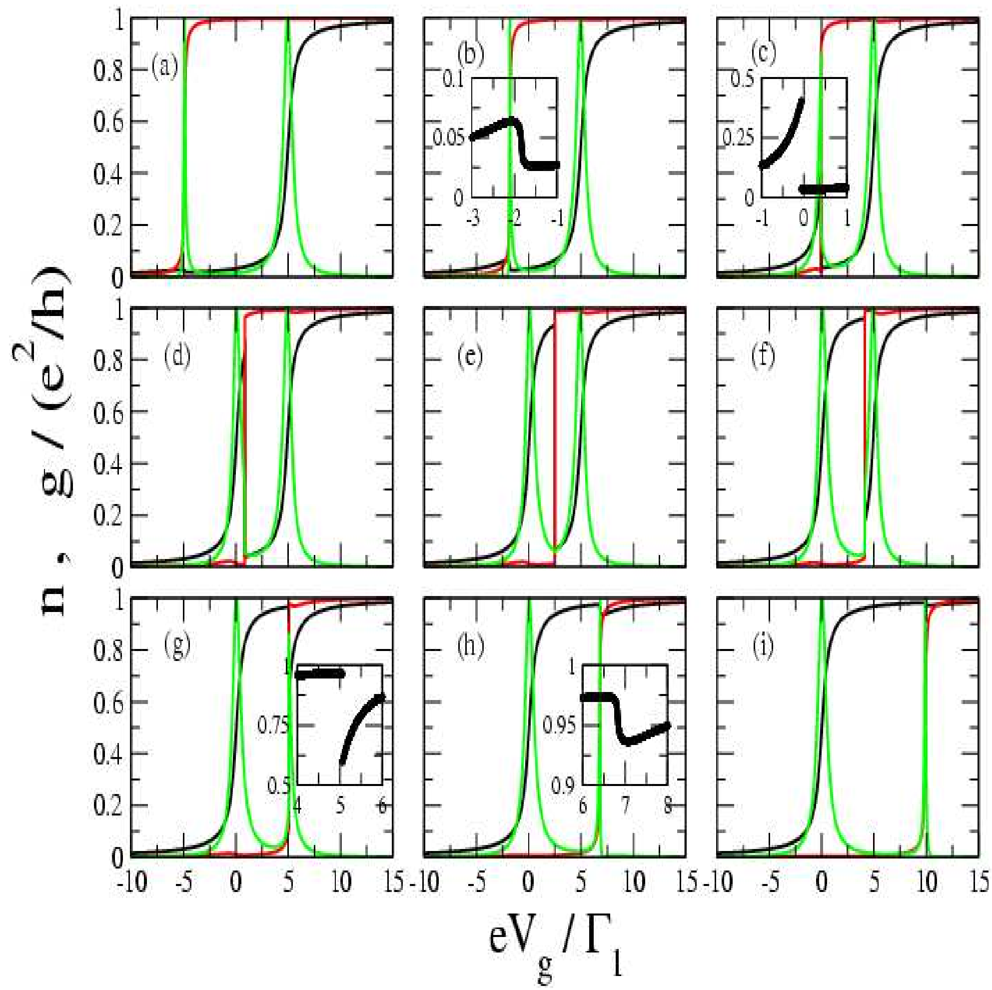


FIG. 4: Level occupations (level 1 - black line; level 2 - red line) and conductance (green line) of a two-level interacting dot at zero temperature. The two levels are connected in the minus configuration. In all the graphs, $\epsilon_1/\Gamma_1 = 0.0$, $\Gamma_2/\Gamma_1 = 0.2$ and $U/\Gamma_1 = 5.0$ while $\epsilon_2$ varies: (a) $\epsilon_2/\Gamma_1 = -5.0$; (b) $\epsilon_2/\Gamma_1 = -2.0$; (c) $\epsilon_2/\Gamma_1 = -0.5$; (d) $\epsilon_2/\Gamma_1 = -0.2$; (e) $\epsilon_2/\Gamma_1 = 0.0$; (f) $\epsilon_2/\Gamma_1 = 0.2$; (g) $\epsilon_2/\Gamma_1 = 0.5$; (h) $\epsilon_2/\Gamma_1 = 2.0$; (i) $\epsilon_2/\Gamma_1 = 5.0$. The insets to panels (b), (c), (g) and (h) show $n_1$ in black circles in the region of fast variation, showing clearly that in cases (b) and (h) the variation is continuous [like cases (a) and (i)], while in cases (c) and (g) it is discontinuous [like cases (d)–(f)] (to an accuracy in $V_g/\Gamma_1$ better than $10^{-3}$).

## IV. INTERACTION EFFECTS

We now turn on the interactions. We will focus on two-level systems from now on. The simplest effect of the interactions is that a filled level pushes unfilled ones toward higher energies by the Hartree term. However, interactions can lead to much more interesting phenomena, such as non-monotonous population of the levels. In the two limiting cases in terms of the ratio between the widths of the two levels (i.e., one of the levels has zero width, or has the same width as the other level respectively), one finds either of the two most basic effects:

I. As was first noted by Silvestrov and Imry[8], when one of the levels is completely decoupled from the lead (i.e., has zero width), it is either completely filled or completely empty at zero temperature. As the gate voltage is swept from low to high values, the wider level is first filled (if its energy is not too much higher than that of the narrow level), and pushes up the energy of the narrow level. Indeed, for low gate voltage values, filling the wider level gives lower total kinetic energy than filling the narrow one. However, At some point, for higher gate voltage values, the kinetic energy considerations make it advantageous to fill the narrow level instead , thus moving the wider one toward higher energy values, and reducing its population. Thus, at that point there is a sharp jump in the occupation of both levels, and in the conductance. Also, the two conductance peaks result from filling the same level twice, and thus have equal lineshapes.

II. For levels of comparable widths, no discontinuity occurs. As the gate voltage is swept, the two levels start becoming populated. However, if one level

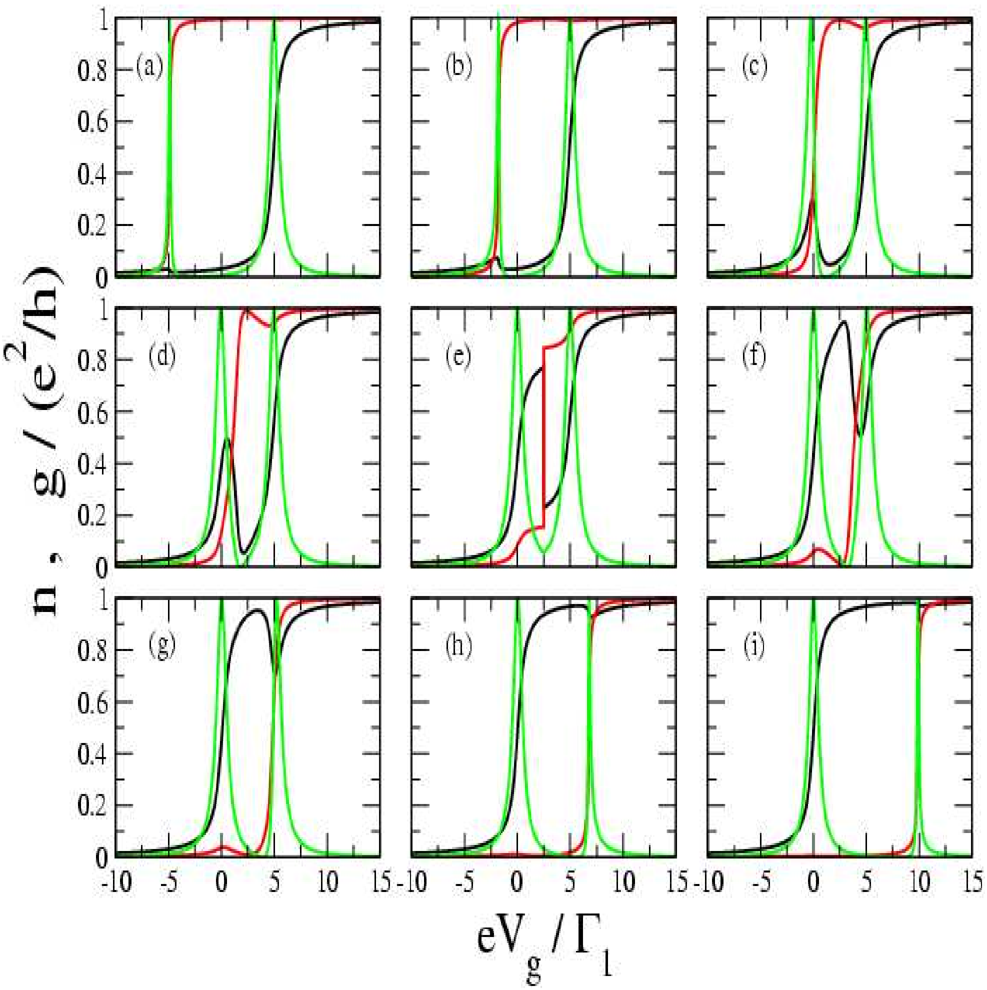


FIG. 5: Level occupations (level 1 - black line; level 2 - red line) and conductance (green line) of a two-level interacting dot at zero temperature. The two levels are connected in the plus configuration. In all the graphs, $\epsilon_1/\Gamma_1 = 0.0$, $\Gamma_2/\Gamma_1 = 0.2$ and $U/\Gamma_1 = 5.0$ while $\epsilon_2$ varies: (a) $\epsilon_2/\Gamma_1 = -5.0$; (b) $\epsilon_2/\Gamma_1 = -2.0$; (c) $\epsilon_2/\Gamma_1 = -0.5$; (d) $\epsilon_2/\Gamma_1 = -0.2$; (e) $\epsilon_2/\Gamma_1 = 0.0$; (f) $\epsilon_2/\Gamma_1 = 0.2$; (g) $\epsilon_2/\Gamma_1 = 0.5$; (h) $\epsilon_2/\Gamma_1 = 2.0$; (i) $\epsilon_2/\Gamma_1 = 5.0$. In this figure there is no discontinuity in any of the cases.

has a lower bare energy, or is wider, this level gets populated faster, and repulses the electrons out of the other level, thus increasing even further its own population. When the gate voltage becomes higher, the process is reversed: the less-populated level starts to be occupied again, and in turn reduces the population of the more-populated level. This effect causes the conductance peaks to be asymmetric. This effect is most pronounced when the level widths are in fact equal.

We will begin by examining the case of levels in the minus configuration. This is the simpler case, since, as we have seen in the non-interacting case, the interference effects do not affect the dot's population. To start with, we give examples to the two limiting cases discussed above in Fig. 3. One can observe that, in contrast with the non-interacting case discussed in the previous section, the conductance does not go to zero in both cases - in the first, one level is completely decoupled from the rest of the system (except for the interaction), so no interference can occur even in the conductance. In the second case, the levels have equal widths, and $\epsilon_{-,v}$ goes to infinity (See Eq. (12)).

In intermediate cases between those two limits, all kinds of combinations of these two phenomena can occur. Some typical cases are shown in Fig. 4. In all those cases the interaction is much stronger than the level widths, and the width of level 2 is much smaller than the width of level 1, but the distance between the two levels varies.

The most interesting feature of the results is that the phenomena of discontinuity of the dot's properties (level populations and conductance) as a function of $V_g$ is not restricted to the case of a level of zero width shown above, but can appear even when the widths of both levels are finite. As one can see in the figure, the discontinuity occurs when the energies of the levels are sufficiently close [cases (c)–(g)]; otherwise, the variation is continuous. By varying the other parameters we have found that for any

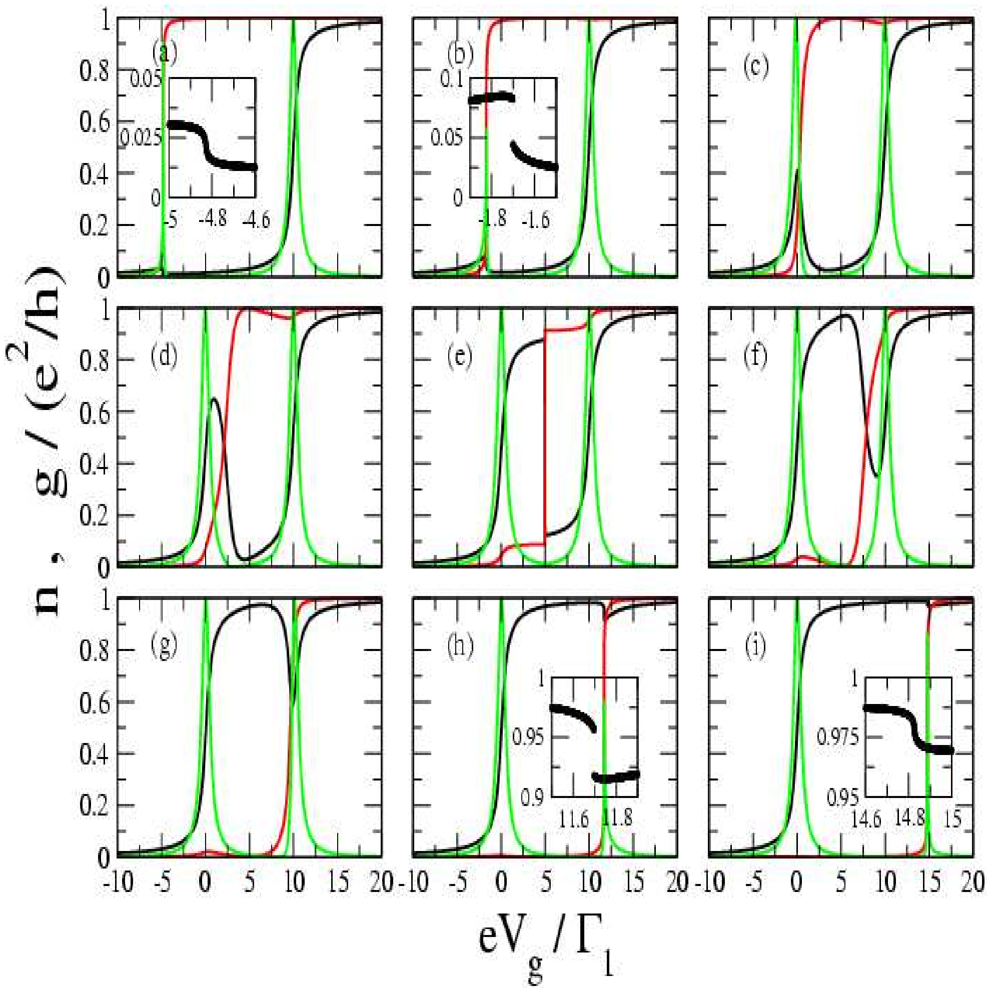


FIG. 6: Level occupations (level 1 - black line; level 2 - red line) and conductance (green line) of a two-level interacting dot at zero temperature. The two levels are connected in the plus configuration. In all the graphs, $\epsilon_1/\Gamma_1 = 0.0$, $\Gamma_2/\Gamma_1 = 0.1$ and $U/\Gamma_1 = 10.0$ while $\epsilon_2$ varies: (a) $\epsilon_2/\Gamma_1 = -5.0$; (b) $\epsilon_2/\Gamma_1 = -2.0$; (c) $\epsilon_2/\Gamma_1 = -0.5$; (d) $\epsilon_2/\Gamma_1 = -0.2$; (e) $\epsilon_2/\Gamma_1 = 0.0$; (f) $\epsilon_2/\Gamma_1 = 0.2$; (g) $\epsilon_2/\Gamma_1 = 0.5$; (h) $\epsilon_2/\Gamma_1 = 2.0$; (i) $\epsilon_2/\Gamma_1 = 5.0$. The insets to panels (a), (b), (h) and (i) show $n_1$ in black circles in the region of fast variation. One can see the variation is continuous in all cases except (b) and (h), where it is discontinuous (to accuracy in $V_g/\Gamma_1$ better than $10^{-3}$).

given value of level separation (including zero), this effect occurs if the interaction is strong enough, and the ratio between the width of the narrow level and the width of the wide level is small enough — The limiting values are less restrictive for close levels, and more demanding for far-away ones.

In addition to this effect, the second, continuous effect of non-monotonous level filling can also be observed in cases (c)–(g). However, it is quite weak here, since the level widths are far from being equal.

Considering the conductance, we have seen in the non-interacting case that it goes to zero at a value of $V_g$ on the narrower peak side away from the wider peak. This effect is manifested only when there is no discontinuity, and results in an asymmetry of the narrower peak. In cases (c)–(g), the discontinuity skips over this point, but leaves the narrow peak asymmetric. In addition, since the wider level is filled in both the conductance peaks, it makes the narrow peak wider in comparison with the non-interacting case (Although, in contrast with the case of Fig. 3(b), the narrow level has a finite width, and the two conductance peaks have *different* lineshapes).

The situation is, however, quite different in the plus configuration. Here, there is a strong interference effect on the populations of the two levels. This is due to both the off diagonal element of the total widths matrix Γ, (which create imaginary off diagonal elements in the dot's inverse Green function), and the Fock term (which create real off diagonal elements in the dot's inverse Green function). Both these terms are absent in the minus configuration discussed above.

Fig. 5 shows the results in the plus configuration, where all parameters values are the same as in Fig. 4. Because of the interference effects on the populations of the two

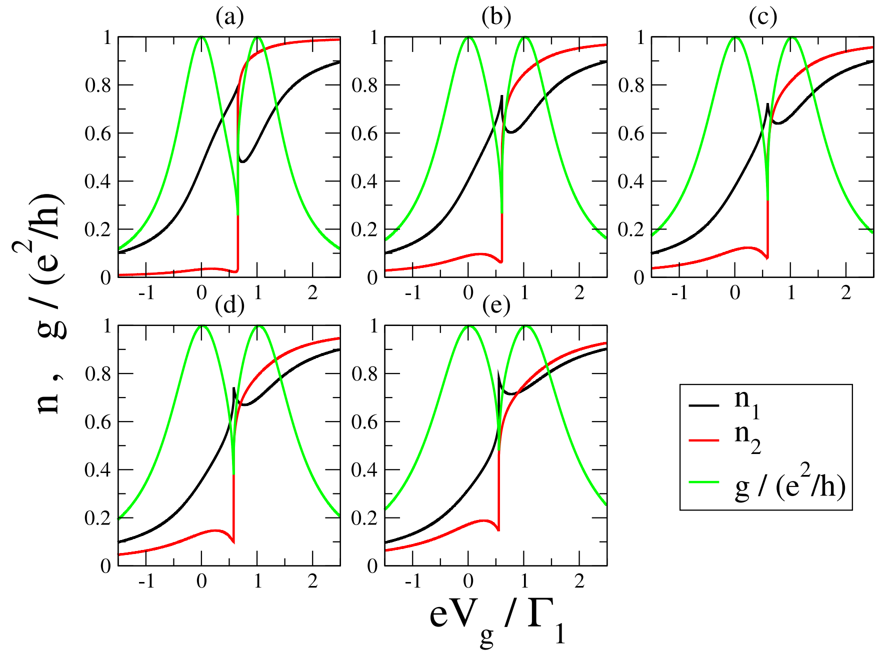


FIG. 7: Level occupations and conductance of a two-level interacting dot at zero temperature. The two levels are connected in the *plus* configuration. In all the graphs, $\epsilon_1/\Gamma_1 = 0.0$, $\epsilon_2/\Gamma_1 = 0.1$ and $U/\Gamma_1 = 1.0$ while $\Gamma_2$ varies: (a) $\Gamma_2/\Gamma_1 = 0.1$; (b) $\Gamma_2/\Gamma_1 = 0.3$; (c) $\Gamma_2/\Gamma_1 = 0.4$; (d) $\Gamma_2/\Gamma_1 = 0.5$; (e) $\Gamma_2/\Gamma_1 = 0.7$. In cases (a) and (b) $n_1$ increases at the discontinuity, in case (c) it does not change, while in cases (d) and (e) it decreases at the discontinuity. In all the cases, $n_2$ increases at the discontinuity.

levels, there are no discontinuities here, except in the case of exactly degenerate levels [case (e)], where we observe the *non-interacting discontinuity*, which occurs even for free electrons (as we have seen in Fig. 1(d) — This point will be discussed more fully later on).

Instead of discontinuities we observe in Fig. 5 a continuous version of effect I, where the narrower level depopulates the wider one as $V_g$ is increased (like, e.g., case (d) for $V_g/\Gamma_1$ near zero), resulting in a broadening of the of the narrow conductance peak. We also observe effect II, where the inverse occurs (such as, e.g., case (f) for $V_g/\Gamma_1$ near zero), contributing to the asymmetry of the wide peak.

We also note that here, in all the cases [except the exactly degenerate case (e)] there is a value of $V_g$ between the two conductance peaks where the conductance goes to zero, as for the non-interacting case.

Nevertheless, we can obtain discontinuities even in the plus configuration. This is exemplified in Fig. 6, in which the parameters are similar to Fig. 5, but the interaction is stronger and the ratio between the narrow level width and the wide level width is smaller. As in the minus case, there is no discontinuity when the levels are too far away [cases (a) and (i)]. In contrast with the minus case, interference effects prevent the discontinuities when the levels are too close [cases (c)–(g), except the non-interacting discontinuity for the exactly degenerate case (e)]. Only for the intermediate cases (in terms of energy levels distance) does discontinuity occurs [as can be seen in the insets to panels (b) and (h)].

In addition, continuous non-monotonicity of the level populations (and the resulting broadening and asymmetry of the narrow peak) occurs in cases (c), (d), (f) and (g), in a similar way to the corresponding cases in Fig. 5. Here too the conductance vanishes for some value of $V_g$ between the two conductance peaks in all cases [except (e)]. This happens even in the discontinuous cases [in contrast with the situation in the minus configuration, Fig. 4(c)–(g)]. The reason is the smallness of the discontinuity even when it occurs.

In Sec. III we have seen that for a non-interacting dot in the plus configuration, when the two levels are almost degenerate, they can be treated as a linear combination of a wide and a very narrow effective levels, almost decoupled for each other. The presence of the narrow effective level causes a sharp variation in the population of the dot's original levels as a function of $V_g$. In the limit of exactly degenerate levels, the narrow level width become zero (it becomes completely decoupled), so a discontinuity occurs[4,10].

The results shown so far seem to imply that in the presence of interaction this sharp variation disappears, except

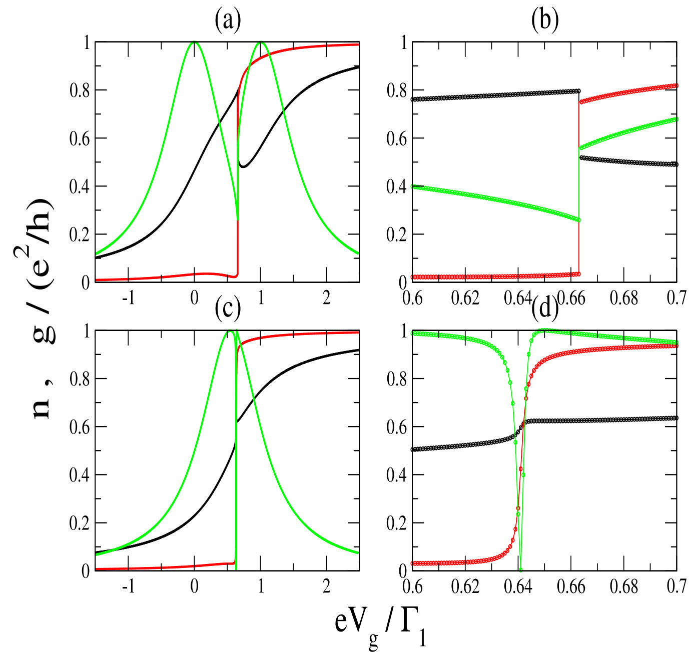


FIG. 8: Level occupations (level 1 - black line; level 2 - red line) and conductance (green line) of a two-level dot at zero temperature. The two levels are connected in the plus configuration. In all the graphs, $(\epsilon_2 - \epsilon_1)/\Gamma_1 = 0.1$ and $\Gamma_2/\Gamma_1 = 0.1$. (a-b) $\epsilon_1/\Gamma_1 = 0.0$, $U/\Gamma_1 = 1.0$ - panel (b) is a close-up on the sharp features of panel (a); (c-d) $\epsilon_1/\Gamma_1 = 0.55$, $U/\Gamma_1 = 0.0$ - panel (d) is a close-up on the sharp features of panel (c). In the non-interacting case the variation is very sharp but continuous; in the interacting case there is a discontinuity.

for the case of coinciding levels, where the non-interacting discontinuity is still observed. However, This is only true for strong interactions, which generate a strong Fock interference term between the levels. For weak interactions (too weak for discontinuities at intermediate level separations to occur), the situation is quite different. Here, because of the presence of the effective narrow level, the interactions can turn the sharp but continuous variation of the level populations in the non-interacting case into a discontinuous one. The jump actually occurs for the effective levels, increasing the population of the narrow effective level by almost one, and reducing the population of the wider effective level by a smaller amount (since the interaction is relatively weak).

A typical situation is exhibited in Fig. 7. Here the first dot level width, the level distance and interaction are fixed, but the second dot level width varies. When the second dot level is much narrower than the wide one [cases (a) and (b)], the picture is quite similar to the usual interacting discontinuity – at the discontinuity the population of the narrow dot level rises, while that of the wide dot level falls. This is because the narrow dot level is composed mainly of the narrow effective level, while the wide dot level is composed mainly of the wide effective level. When the narrow dot level width is comparable to the of the wider dot level [cases (d) and (e)], the results resemble the non-interacting discontinuity – the occupations of both the wider and the narrower dot levels rise at the discontinuity. This happens since the wider dot level now has a larger share in the narrow effective level, and, as was explained above, the increase in the population of the narrow effective level is larger than the (absolute value of the) decrease in the population of the wide effective level. There is an intermediate value of the narrow dot level width [case (c)] where only the narrower dot level population jumps, while the wider dot level population is continuous, since the effects of the wide and narrow effective levels on its population exactly cancel.

Due to the large discontinuities in these cases, the conductance does not vanish between the two peaks in any of the cases considered. The result is two wide and overlapping conductance peaks, with discontinuous features in the conductance valleys between them.

To clarify the above points, in Fig. 8 we compare the results with and without interaction for parameter values corresponding to Fig. 7(a). It can be clearly seen that although in the non-interacting case the variation of the physical parameters (especially the conductance) with $V_g$ is very fast, it is still continuous, and discontinuities can appear only with the addition of interactions.

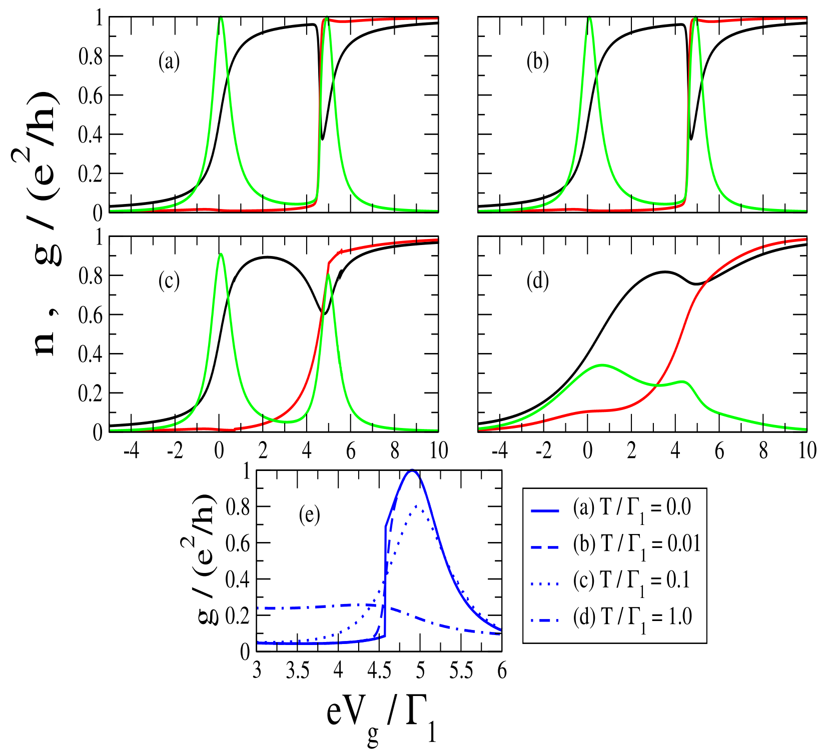


FIG. 9: Level occupations (level 1 - black line; level 2 - red line) and conductance (green line) of a two-level dot at various temperatures. The two levels are connected in the minus configuration. In all the graphs, $\epsilon_1/\Gamma_1 = 0.0$, $\epsilon_2/\Gamma_1 = 0.3$, $\Gamma_2/\Gamma_1 = 0.2$, and $U/\Gamma_1 = 5.0$ (a) $T/\Gamma_1 = 0.0$; (b) $T/\Gamma_1 = 0.01$; (c) $T/\Gamma_1 = 0.1$; (d) $T/\Gamma_1 = 1.0$; (e) shows the conductance curves in the different temperatures together.

Finally we remark on the effects of finite temperatures. In Fig. 9 we examine one particular case (having parameter values intermediate between those of Fig. 4(c) and Fig. 4(d)). For temperatures lower than the narrow level width, the only effect of the temperature is to make the discontinuity smooth. Higher temperatures cause the smearing of the entire curves, and the lowering of the conductance peaks heights below the maximal value of $e^2/h$.

Thus, discontinuities may appear experimentally as fast gate voltage dependence of the physical parameters, which thus show temperature dependence for temperatures much lower than the, e.g., conductance peaks widths. Of course, one cannot differentiate experimentally between discontinuous features and continuous features having width smaller than the lowest accessible temperature.

## V. CONCLUSIONS

In this paper we examined some of the various phenomena which may occur in a quantum dot where both interaction effects and inter-level interference effects are important. We now turn to summarize our results.

We have first shown that the occurrence of more conductance peaks than energy levels in the dot can happen even in the non-interacting case, and may help explain recent experimental observations.

In the interacting case we have found that in the minus configuration, where the interference between the two levels does not affect their populations, discontinuities occur if the levels are close enough, the interaction is strong enough, and the ratio of the level widths is much different from unity. In contrast, in the plus configuration interference effects are important. In the strong interaction regime discontinuities can only occur when the levels are not too far away but not too close; again, the widths ratio needs to be significantly different from one. In the weak interactions regime, the fast variation of the population in the non-interacting case for almost

degenerate levels can lead to discontinuities in the interacting case even for comparable widths. These results agree with the "phase diagram" picture of Golosov and Gefen[16] in the overlapping part of the parameter space.

In both configurations, even when no discontinuity occurs, there is usually a continuous version of mechanism I of non-monotonous filling, accompanied by a broadening of the narrow conductance peak. In addition, if the levels are not too far apart, the continuous or discontinuous type I non-monotonicity is accompanied by type II non-monotonous behavior, causing asymmetry of the conductance peaks.

In either the plus or minus case, when no discontinuity occurs, or when the discontinuity is weak enough, there is a conductance zero in a location similar to the non-interacting case. Strong enough discontinuities can cause the conductance zero to be skipped.

Finite temperatures smear the discontinuities. The latter leave their mark as sharp features in the gate voltage dependence of the different physical properties, which show very strong temperature dependence relative to other parts of the gate voltage dependence curves.

We conclude with a final remark. Our result in the interacting case were obtained using the self-consistent Hartree-Fock approximation, which neglects correlation effects. These may reduce the parameter space regime in which discontinuities occur, or even eliminate it completely. It can be expected, however, that the various continuous behaviors found will remain even in a more complete theory.

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